1-Heptanethiol

Other names:	1-Heptylthiol
	HEPTYLTHIOL
	Heptyl mercaptan
	Heptyl thiol
	N-HEPTYL MERCAPTAN
	Normal-heptyl mercaptan
	USAF EK-2122
	heptane-1-thiol
	n-Heptylmercaptan
Inchi:	InChI=1S/C7H16S/c1-2-3-4-5-6-7-8/h8H,2-7H2,1H3
InchiKey:	VPIAKHNXCOTPAY-UHFFFAOYSA-N
Formula:	C7H16S
SMILES:	CCCCCCCS
Mol. weight [g/mol]:	132.27
CAS:	1639-09-4

Physical Properties

Property code	Value	Unit	Source
chl	-5442.97 ± 0.75	kJ/mol	NIST Webbook
gf	37.45	kJ/mol	Joback Method
hf	-149.50 ± 0.96	kJ/mol	NIST Webbook
hfl	-200.50 ± 0.92	kJ/mol	NIST Webbook
hfus	17.93	kJ/mol	Joback Method
hvap	51.00	kJ/mol	NIST Webbook
hvap	50.60 ± 0.20	kJ/mol	NIST Webbook
log10ws	-2.82		Crippen Method
logp	2.887		Crippen Method
mcvol	125.840	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
rinpol	1055.00		NIST Webbook
rinpol	1013.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	1024.00		NIST Webbook

rinpol	1024.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1031.00		NIST Webbook
ripol	1248.70		NIST Webbook
ripol	1267.00		NIST Webbook
ripol	1256.00		NIST Webbook
ripol	1253.80		NIST Webbook
ripol	1267.00		NIST Webbook
sl	375.35	J/mol×K	NIST Webbook
tb	447.65	K	KDB
tb	450.20	K	NIST Webbook
tb	450.05 ± 0.30	K	NIST Webbook
tb	445.00 ± 2.00	K	NIST Webbook
tc	609.58	K	Joback Method
tf	229.80 ± 0.50	K	NIST Webbook
tf	229.80 ± 0.30	K	NIST Webbook
tt	229.93 ± 0.08	K	NIST Webbook
tt	229.92 ± 0.02	K	NIST Webbook
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.38	J/mol×K	609.58	Joback Method
cpg	291.46	J/mol×K	547.19	Joback Method
cpg	302.15	J/mol×K	578.38	Joback Method
cpg	243.63	J/mol×K	422.42	Joback Method
cpg	256.37	J/mol×K	453.61	Joback Method
cpg	268.58	J/mol×K	484.81	Joback Method
cpg	280.27	J/mol×K	516.00	Joback Method
cpl	259.32	J/mol×K	298.15	NIST Webbook
cpl	259.32	J/mol×K	298.15	NIST Webbook
hfust	25.40	kJ/mol	229.90	NIST Webbook
hfust	25.38	kJ/mol	229.92	NIST Webbook
hfust	25.40	kJ/mol	229.90	NIST Webbook
hvapt	45.00	kJ/mol	422.50	NIST Webbook
hvapt	49.50	kJ/mol	309.00	NIST Webbook
sfust	110.40	J/mol×K	229.92	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	447.70	K	102.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54403e+01
Coeff. B	-4.15483e+03
Coeff. C	-6.62750e+01
Temperature range (K), min.	340.47
Temperature range (K), max.	476.47

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.92087e+01
Coeff. B	-9.41115e+03
Coeff. C	-1.22765e+01
Coeff. D	6.51592e-06
Temperature range (K), min.	229.92
Temperature range (K), max.	645.00

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol1840.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1639094&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1840

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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